TN 295
.U4
IC-8811
1980

IC 8811

Bureau of Mines Information Circular/1980

LIBRARY OF CONGRESS
4
EXCHANGE AND GIFT

Methodology for Evaluating Integral Gaussian Profiles

By Arthur B. Campbell III

UNITED STATES DEPARTMENT OF THE INTERIOR

Information Circular 8811

Methodology for Evaluating Integral Gaussian Profiles

By Arthur B. Campbell III

UNITED STATES DEPARTMENT OF THE INTERIOR
Cecil D. Andrus, Secretary

BUREAU OF MINES
Lindsay D. Norman, Acting Director

TN
295
.U4
I.C.-8811, 1958

This publication has been cataloged as follows:

Campbell, Arthur Benedict III, 1943-
Methodology for evaluating integral Gaussian profiles.

(Information circular - U.S. Bureau of Mines ; 8811)

Bibliography: p. 14-15.

1. Solids, Effect of radiation on—Data processing. 2. Ion bombardment—Data processing. 3. X-ray spectroscopy—Data processing. 4. Sputtering (Physics)—Data processing. I. Title. II. Title: Integral Gaussian profiles. III. Series: United States. Bureau of Mines. Information circular ; 8811.

TN295.U4 [QC176.8.R3] 622'.08s [669'.94] 79-19923

CONTENTS

	Page
Abstract	1
Introduction	1
Experimental techniques	2
Use of ABC10 program	5
Example	9
Conclusions	13
References	14
Appendix.--Listing of ABC10	16

ILLUSTRATIONS

1. Integral data for nickel implanted into iron at 25 kev expressed as Ni-L X-ray yield versus sputtering charge 9
2. Profiles obtained for nickel implanted into iron at 25 kev as obtained using ABC10 12

TABLES

1. Symbols used in ABC10 6
2. Output of computer and input of data for evaluation of integral profiles for nickel implanted into iron at 25 kev and for obtaining profiles for as-implanted case 10
3. Output of computer and input of data for evaluation of integral profiles for nickel implanted into iron at 25 kev and for obtaining profiles for annealed case 11
4. Values of range and range straggle for 30-kev As^{+} implanted into silicon as determined from data of Ludvik, LSS theory, Iwaki, and the PIXE-IS technique using ABC10 13

METHODOLOGY FOR EVALUATING INTEGRAL GAUSSIAN PROFILES

by

Arthur B. Campbell III[1]

ABSTRACT

This Bureau of Mines report describes a method that utilizes a computer program to evaluate integral Gaussian profiles of atomic concentration versus depth in a solid. The specific use illustrated involves profiling ion-implanted metals using proton-induced X-ray emission (PIXE) analysis and ion sputtering (IS) for sectioning.

INTRODUCTION

As part of the Bureau of Mines effort to minimize the requirements for minerals through conservation and substitution, an investigation of ion-implanted alloys was initiated in 1975. These alloys are an integral part of the bulk material, down to depths of about 1000 A, and as such do not have the interfacial bonding disadvantages inherent at the junction between substrates and coatings. These ion-implanted alloys have been shown to be as corrosion resistant as comparable bulk alloys in certain applications (4-5)[2], while using orders of magnitude less alloying material and thus realizing a considerable conservation. This is especially important since common alloys include such strategic elements as chromium and nickel. As a first step in understanding how ion-implanted alloys resist corrosion, a study was initiated into the physical properties of ion-implanted metals. The distribution of elements below the surface was included in this study, which used proton-induced X-ray emission (PIXE) analysis combined with sectioning via ion sputtering (IS).

The PIXE-IS depth-profiling technique provides data that are in an integral form; that is, they represent elemental concentration (areal) below a certain depth versus depth. To convert these data to the more useful form of a differential profile of concentration (volume) versus depth, a computer program has been developed that produces this depth profile from the integral data.

---

[1] Research physicist, Avondale Research Center, Bureau of Mines, Avondale, Md.

[2] Underlined numbers in parentheses refer to items in the list of references preceding the appendix.

When actually in use or for intentional redistribution of elements, ion-implanted alloys may be subjected to thermal treatments that will alter these profiles, so in addition to profiles of as-implanted alloys, it is also necessary to obtain profiles of alloys that have been annealed. This same computer program includes this capability.

This Information Circular describes a computerized method for evaluating integral Gaussian profiles. It includes enough of the basic theory of ion implantation and diffusion that is behind the program so that the usefulness of this program to other researchers can be seen.

EXPERIMENTAL TECHNIQUES

A brief summary of the theories of ion implantation profiles and diffusion and the PIXE-IS technique will better explain the use of this program.

Ion implantation involves the bombardment of a solid with accelerated ions having energies typically in the tens of kiloelectronvolts. These ions lose energy in traversing the solid through interactions with the electrons and nuclei of the solid, and their final stopping point is determined statistically. The most successful theory of ion implantation is that of Lindhard, Scharff, and Schiott (LSS)(12), which has undergone many updatings and modifications (16) but is still the same basic statistical system. To a good approximation (±20 percent), the profile of ion-implanted atoms in a solid such as a semiconductor or a metal can be described as

$$y(x) = y_o \exp\left[\frac{-(x - R_p)^2}{2(\Delta R_p)^2}\right], \tag{1}$$

where $y(x)$ is the concentration in atoms/cm^3 of the implanted element at a depth x, y_o is the maximum concentration, R_p is the projected range or most probable depth, and ΔR_p is the range straggle or standard deviation in the range. This equation is valid for implantation at normal incidence to the surface of the solid where R_p, the range projected along the beam direction, will be measured perpendicular to the surface. The LSS theory is strictly applicable only in the case of an amorphous solid, that is, in the absence of inhomogeneities such as grain boundaries.

To predict the effect of heat treatment or annealing on the profile as given by equation 1, Fick's law of diffusion (6) is used. Mathematically it is expressed as

$$\frac{\partial y(x,t)}{\partial t} = D \frac{\partial^2 y(x,t)}{\partial x^2}, \tag{2}$$

where $y(x,t)$ is the concentration as a function of depth after annealing for a time t, where the diffusion coefficient is D in cm^2/sec.

A solution to equation 2, assuming a semi-infinite solid with no losses at the surface, is (3)

$$y(x,t) = \frac{1}{\sqrt{\pi}} \int_{\frac{-x}{2\sqrt{Dt}}}^{\infty} y(x + 2\eta\sqrt{Dt}) \exp(-\eta^2) d\eta + \frac{1}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{\infty} y(-x + 2\eta\sqrt{Dt}) \exp(-\eta^2) d\eta , \tag{3}$$

where $y(x,o) = y(x)$ and η is simply a variable of integration. Integrating equation 3, one obtains

$$y(x,t) = (y_o/2)\, y_1^{-\frac{1}{2}} (y_2 + y_3) , \tag{4}$$

where

$$y_1 = 1 + \frac{2Dt}{(\Delta R_p)^2} \tag{5}$$

$$y_2 = \exp\left[\frac{-(x - R_p)^2}{2(\Delta R_p)^2 y_1}\right] \operatorname{erfc}\left[\frac{-x(\Delta R_p)^2 - 2R_p Dt}{2(\Delta R_p)^2\sqrt{Dt}\sqrt{y_1}}\right] \tag{6}$$

$$y_3 = \exp\left[\frac{-(x + R_p)^2}{2(\Delta R_p)^2 y_1}\right] \operatorname{erfc}\left[\frac{x(\Delta R_p)^2 - 2R_p Dt}{2(\Delta R_p)^2\sqrt{Dt}\sqrt{y_1}}\right] \tag{7}$$

where erfc is the complementary error function. Note that equation 4 is finite as both x and t approach infinity. It can be seen that equation 4 reduces to equation 1 for t = o. Since we have assumed an impenetrable barrier at the surface, y_o can be defined from the definition of ϕ, the implanted fluence (or dose), in atoms/cm^2.

$$\phi = \int_o^{\infty} y(x,o)dx. \tag{8}$$

With a change of variable and including equation 4, this becomes

$$y_o = \frac{\phi}{\sqrt{2}(\Delta R_p)} \left[\int_{\frac{-R_p}{\sqrt{2}(\Delta R_p)}}^{\infty} \exp(-z)^2 dz\right]^{-1} = \frac{2\phi}{\sqrt{2\pi}(\Delta R_p)} \left[1 + \operatorname{erf}\left(\frac{R_p}{\sqrt{2}(\Delta R_p)}\right)\right], \tag{9}$$

where erf is the error function.

Putting this into equation 4

$$y(x,t) = \frac{\phi}{\sqrt{2\pi}(\Delta R_p)} \left[1 + \operatorname{erf}\left(\frac{R_p}{\sqrt{2}(\Delta R_p)}\right)\right] y_1^{-\frac{1}{2}} (y_2 + y_3) , \tag{10}$$

which is the complete solution.

The PIXE-IS technique involves the use of ion beams for both analysis and sectioning. Beams of high-energy (100- 200-kev) protons bombarding the surface produce X-rays characteristic of the elements present in a thin surface layer ($\simeq$1000 to 5000 A). These X-rays can also be used to obtain quantitative information (14). Thus, it is possible to obtain a conversion from X-ray yield (X-ray photons measured per microcoulomb of proton beam) to areal concentration (atoms of element per square centimeter of surface). For thin enough films (11) and with a knowledge of the density of the film, atomic concentrations (in atoms per cubic centimeter) can be obtained.

Low-energy ($\simeq$1 kev) inert gas ions can interact with a surface such that atoms of the surface are ejected. This process of physical sputtering is used to controllably remove thin layers from the surface, even as thin as one atomic layer. This process can thus be used to depth-profile a surface.

The profiles obtained by the PIXE-IS technique are of an integral form; that is, they are a measure of the integral areal concentration or amount left in the surface versus depth. The process involves measuring via PIXE the X-ray photons per microcoulomb of a particular element, sputtering for a particular charge (microcoulombs) of inert gas ions, and then remeasuring the X-ray yield. The difference in the X-ray yields is a measure of the amount of the element removed by sputtering, assuming the PIXE analysis depth is greater than the profile depth. There will be a limitation from this factor on profiles that are deeper than about 5000 A, which could be important for the case of long anneal times. With appropriate conversion factors, the data obtained (X-ray yield versus sputtering charge) can be converted to areal concentration versus depth.

The conversion from X-ray yield to areal concentration is accomplished using the thin-film approximation (11),

$$T = I/\sigma_x \ , \tag{11}$$

where T is the areal concentration in atoms/cm^2, I is the X-ray yield, and σ_x is the X-ray production cross section. The conversion from sputtering charge is accomplished using the equation

$$d = QCSf_a/[A_p(1 + \gamma)] \ , \tag{12}$$

where d is the depth normal to the surface, Q is the accumulated sputtering charge, C is a unit conversion factor, S is the sputtering yield in atoms sputtered per ion, f_a is a geometrical factor, A_p is the area of the proton analysis beam, and γ is the secondary electron emission coefficient during sputtering. These factors are measured during preliminary PIXE and IS experiments.

To convert this integral data to a differential profile of atomic concentration versus depth, a method had to be developed that would produce a physically realistic profile from these data points. Since theoretical predictions are for a Gaussian profile shape (equation 1), it was decided to use the integral of equation 1 and compare this smooth curve with the data using the values of R_p and ΔR_p as parameters for obtaining the best agreement.

In converting the data from annealed samples, it was decided to use the predictions of Fick's law for diffusion of an initially Gaussian profile. Since equation 4 reduces to equation 1 for t = 0, the integral of equation 4

$$N(d,t) = \int_{d}^{\infty} y(x,t)dx \,, \tag{13}$$

where N(d,t) represents the concentration of an element below a depth d, can be used for both as-implanted and annealed samples.

The integral of equation 4 is accomplished using an approximation for the complementary error function (1) and a numerical integration using the method of Gaussian quadrature (7).

The complementary error function can be expressed as

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z) \,, \tag{14}$$

and the approximation

$$\mathrm{erf}(z) \simeq 1 - [a_1 b + a_2 b^2 + a_3 b^3] \exp(-z^2) \tag{15}$$

with $b = 1/(1 + (0.47047)z)$, $a_1 = 0.3480242$, $a_2 = -0.0958798$, and $a_3 = 0.7478556$ (1) is used for $0 \leq z < \infty$ with an accuracy of

$$\mathrm{erf}(z) - \{1 - [a_1 b + a_2 b^2 + a_3 b^3] \exp(-z^2)\} \leq 2.5 \times 10^{-5} \tag{16}$$

to evaluate equation 13.

The General Services Administration's RAMUS time-sharing computer service has been used for these evaluations, and it provides a program for numerical integration using the Gaussian quadrature method called NUMINT*** (8), which was modified for use and is included in this program, as shown in the appendix.

USE OF ABC10 PROGRAM

A runthrough of the program, which was entitled ABC10, will serve to explain its workings and aid in understanding how to use it. All line numbers refer to those in the ABC10 program printed in the appendix. Note that the computer language BASIC is used. In this section we will refer to the symbols as they would appear in the printout during actual use of the program.

In the use of the program, one must first have a graph of the integral profile data points. Initializing parameters are first entered into the program, and then intelligent estimates are made as to the values of range (R) and range straggle (RS), and diffusion coefficient (D) in the case of an annealed profile. The resulting profile values are compared with the data until the best agreement is reached. This method is fitting by inspection. Once the best agreement by this method has been reached, one would stop and draw a detailed plot of the computer-generated curve on the same graph that

contains the data points. If the two look similar, a detailed manual analysis must be performed to obtain an estimate of the standard deviation. In all cases, this method was able to produce integral profiles that agreed with the data to no worse than 10 percent standard deviation.

The initial steps of the program provide for the input of constants and data to be used in the evaluations. Table 1 lists the symbols typed out during operation, but note that these do not necessarily conform to the notation used in the program because of expediencies in programing. The symbols are defined later in the text. Statement 120 is a comment that appears first in the operation of the program and provides a way of resetting the program during use by using certain nonrealistic values of range and range straggle. In the normal operation of the program, various values of R, R.S., and D are chosen; the resultant integral function is compared with the data, and the values that produce the best fit are chosen. In some cases, it is necessary to reset the initial parameters, and statement 120 provides the user with a reference to the resulting procedure.

TABLE 1. - Symbols used in ABC10

Definition (text)	Symbol in print	Symbol in program
Range (R_p)	R	B
Range straggle (ΔR_p)	R.S.	C
Diffusion coefficient (D)	D	D
Diffusion time (t)	T	T
Conversion factors:		
Angstroms/10^3 microcoulomb	A/K	K
Atoms/cm^2/photon/microcoulomb	A/C/P/MIC.	H
Incremental depth	STEP SIZE	T6
Infinity (maximum depth ÷ 1.25)	MAXIMUM DEPTH	V
X-ray absorption factor $\left(\frac{\mu}{\rho}\rho\right)$	X-RAY ABSORPTION FACTOR (ANG.-1)	Q8
Stopping power	P	G1
Power factor	F	G2
Initial proton energy	EO	G3

The initial parameters entered are the step size and maximum depth: that is, the incremental step between integral data points desired and the largest depth for an integral data point. This maximum depth is the depth where the integral data points reach an asymptotic value. This is not necessarily zero because of the nature of the sputtering technique (so called knock-on effects or differential sputtering). In a profiling experiment, the sputtering will always be continued until at least this asymptotic value is reached. This maximum depth is also used to define the upper limit of integration, as discussed later. The step size and maximum depth are usually chosen so that the integral is evaluated for points on the abscissa that agree with the data points.

The next parameters that are requested are the values of the integral data at zero sputtering and after completion of the sputtering. These are expressed as the value of the integral at zero and at infinity, and it may be

necessary to use these two as fitting parameters. For several reasons, including peak background and the physics of the sputtering process (15), the data may not approach zero with continued sputtering but rather approach an equilibrium value. This value would be used as the value at infinity, and the program takes this into account in the fitting.

Also included in this program is a factor that takes into account the absorption of X-rays in the solid. If X-rays are produced at some depth x', then the intensity of the X-rays leaving the surface is

$$I = I_o \exp\left[-\left(\frac{\mu}{\rho}\right)\rho x'\right], \tag{17}$$

where I_o is the intensity of the X-rays as produced, μ is the X-ray absorption coefficient, and ρ is the atomic density of the solid. The program evaluates the effect of this absorption at each depth interval, and the resultant integral profile reflects the profile as it would appear as data; that is, with absorption included. Values of the X-ray absorption coefficient are available in tabular form (9), expressed as $\frac{\mu}{\rho}$. Thus, the program requests the absorption factor, which is the product of $\left(\frac{\mu}{\rho}\right)$ and ρ, expressed as inverse angstroms. This somewhat unusual unit is for ease of programing, since the usual unit is $cm^2/gram \times gram/cm^3$, or inverse centimeters. If negligible absorption is expected or to eliminate this correction factor, a value of zero is entered.

The program also takes into account the changes in X-ray production yields because of the energy loss of the protons in traversing the solid. The stopping power (P), the energy loss of the protons per distance traveled, can be assumed to be a constant in the energy region considered (2), and so the instantaneous energy of the protons is

$$E(x) = EO - Px', \tag{18}$$

where E is the energy of the protons at a depth x'. The best fit to the energy dependence of the X-ray production cross section in the energy region of interest here was found to be a power function. Then the ratio of cross sections at a depth x' and at the surface will provide the correction factor (G),

$$G = \left[\frac{EO - Px'}{EO}\right]^F, \tag{19}$$

where F is the predetermined power factor.

In both the case of absorption and the case of energy decrease, the value of x' chosen for evaluation is one-half the distance from d to infinity. This gives an average correction factor, but since these correction factors are not a strong function of depth, this is considered adequate.

The next step in the program is to enter the loop that provides data points, which are the integral of a Gaussian profile function based on the values of range, range straggle, diffusion coefficient, and diffusion time. If the profile is for an unannealed sample, t is set to zero. Note that a nonzero value of D must be entered even though it is not used.

In normal use, the procedure that is followed from here on for unannealed samples involves choosing various values of R and R.S. and comparing the resultant values of the integral Gaussian with the data points in order to get the best fit. This procedure is best accomplished with a graph of the data in front of the computer operator. For a detailed comparison, the operator must go off line and make careful plots of the integral Gaussian functions on the same graph. Manual statistical analysis at this point is time consuming, but for the one that is the "best" fit it will confirm the visual comparison.

Nothing has been said about units since until one wishes a Gaussian profile, the units are arbitrary. In a PIXE-IS experiment, the abscissa would be sputtering charge in coulombs of inert gas ions and the ordinate would be X-ray photons per microcoulomb of protons. After the best integral Gaussian function has been chosen, conversion factors are used to convert these units to depth and areal density, which become depth and atomic density for the profile. The advantage in leaving the units out until this point is that the program can be applied to other profiling techniques.

In line 1190, it will be noted that five numbers are needed for the input statement. Line 1180 asks for R, R.S., D, T, and "1 for profile." This provides a way of exiting from the loop and producing profile data. Normally when various values of range and range straggle are being tried, any other number except 1 is to be entered as the fifth element. When the number 1 is entered, the program produces the requested profile.

To date, the program has been used to obtain profiles for annealed samples after the range and range straggle have been determined from the unannealed samples. This means that the diffusion coefficient is the only fitting parameter. If a profile has not been obtained from an unannealed sample, the three fitting parameters can make the procedure quite complicated.

The profile data are printed out based on the conversion factors and the values of R, R.S., D, and T. In addition to the atomic concentration (called simply "differential" in the program) and depth, the program provides a conversion to atomic percent (based on iron, our most commonly used base material) and implant dose as measured by PIXE. Note that both of these conversions are based on an integral zero level that was entered at statement 1320 as m.

At this point let us return to the question of the value of infinity used in the integration. The numerical integration is stopped at a large enough value to approximate infinity such that the next incremental increase results in a negligible increase in the integral. This is easy since we are dealing with functions that decrease with d. A separate series of runs was conducted using a variety of values for infinity, and it was found that a value

corresponding to 1.25 times the maximum depth (the largest value of sputtering charge or the point where sputtering was stopped) was more than sufficient. We have also chosen to divide the numerical integration into 50 steps. This was found to be more than enough steps to assure accuracy to within three significant figures. This accuracy is consistent with the experimental accuracy of the typical PIXE-IS experiment; thus, the program with the approximation to the complementary error function and the numerical integration is not the limiting factor.

EXAMPLE

What follows is an example of the use of ABC10 for determining profiles for iron implanted with 25 kev nickel. Figure 1 shows the data as obtained using the PIXE-IS technique by monitoring the Ni-L X-ray yield during 180-kev proton bombardment. Sputtering was performed with 1-kev argon ions. Each data point represents the average of three measurements on three separate samples. The solid lines are drawn as a result of using ABC10 to generate the integral of a Gaussian or a diffused Gaussian that agrees as close as possible with the data.

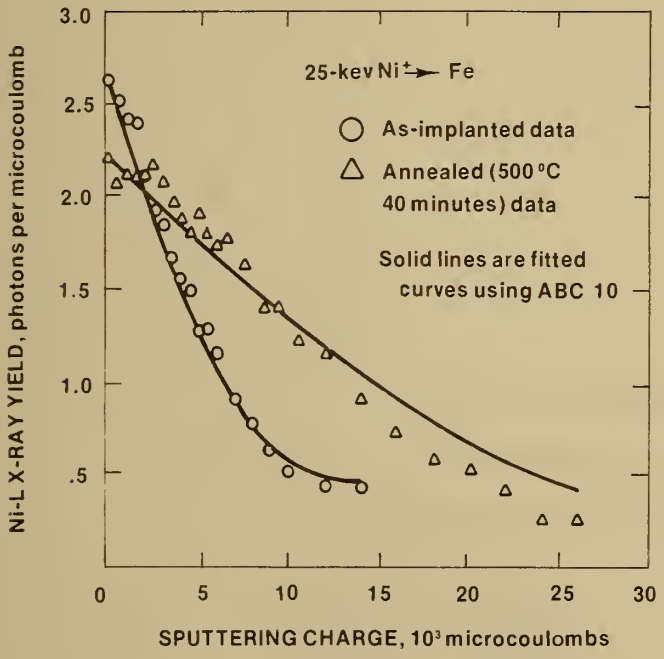

FIGURE 1. - Integral data for nickel implanted into iron at 25 kev expressed as Ni-L X-ray yield versus sputtering charge. The solid lines are curves obtained using ABC10 for fitting.

Table 2 presents the computer output of the curve in figure 1 that represents the as-implanted integral profile and the associated differential concentration profile. It must be emphasized that in this case 15 tries were necessary before this curve was generated and the values for R and R.S. were obtained. After this, the production of the differential profile is almost automatic.

The conversion factors were obtained using equations 11 and 12. Note that the value of 13.4 angstroms per 1,000 microcoulombs can be used to convert range and range straggle to 40.2 angstroms and 53.6 angstroms, respectively.

TABLE 2. - Output of computer and input of data for evaluation of integral profiles for nickel implanted into iron at 25 kev and for obtaining profiles for as-implanted case

```
ENTER VALUE OF INTEGRAL AT 0 AND AT INFINITY? 2.62,.45
ENTER X-RAY ABSORPTION FACTOR (ANG.-1) ? 1E-3
ENTER STOPPING POWER (EV/ANG.), POWER FACTOR, AND EO (EV)
 ? 22.5,2.067,180000
ENTER CONV. FACTORS: A/K AND A/C/P/MIC. ? 13.4,7.4E15
ENTER STEP SIZE, MAXIMUM DEPTH ? 1,14

ENTER R,R.S.,D,T,&1 FOR PROFILE ? 3,4,1,0,0

DEPTH          INTEGRAL
 0              2.62
 1              2.36
 2              2.12
 3              1.85
 4              1.58
 5              1.32
 6              1.09
 7              .896
 8              .745
 9              .633
10              .557
11              .508
12              .48
13              .465
14              .459

ENTER R,R.S.,D,T,&1 FOR PROFILE ? 3,4,1,0,1

DOSE FROM YIELD = 1.81E+16 ATOMS/CM2

DEPTH          DIFFERENTIAL     ATOMIC % (FE)

 0              1.02E+22         12.
13.4            1.19E+22         14.
26.8            1.3E+22          15.4
40.2            1.35E+22         15.9
53.6            1.3E+22          15.4
67.             1.19E+22         14.
80.4            1.02E+22         12.
93.8            8.16E+21         9.62
107.            6.16E+21         7.26
121.            4.37E+21         5.15
134.            2.91E+21         3.43
147.            1.82E+21         2.15
161.            1.07E+21         1.26
174.            5.91E+20         .697
188.            3.07E+20         .362
```

In table 3, the values of R and R.S. obtained from the as-implanted data are used to obtain the curve in figure 1 that is the best match to the annealed data. The value of the diffusion coefficient obtained from this procedure is 5×10^{-18} cm^2/sec.

TABLE 3. - Output of computer and input of data for evaluation of integral profiles for nickel implanted into iron at 25 kev and for obtaining profiles for annealed case

```
ENTER R,R.S.,D,T,&1 FOR PROFILE ? 0,1,1,1,1
ENTER VALUE OF INTEGRAL AT 0 AND AT INFINITY ? 2.2,.25
ENTER X-RAY ABSORPTION FACTOR (ANG.-1) ? 1E-3
ENTER STOPPING POWER (EV/ANG.), POWER FACTOR, AND EO (EV)
 ? 22.5,2.067,180000
ENTER CONV. FACTORS:  A/K AND A/C/P/MIC. ? 13.4,7.4E15
ENTER STEP SIZE, MAXIMUM DEPTH ? 2,26

ENTER R,R.S.,D,T,&1 FOR PROFILE ? 3,4,5E-18,2400,0

DEPTH          INTEGRAL
 0              2.2
 2              1.99
 4              1.82
 6              1.65
 8              1.48
10              1.32
12              1.17
14              1.02
16              .892
18              .772
20              .664
22              .596
24              .487
26              .418

ENTER R,R.S.,D,T,&1 FOR PROFILE ? 3,4,5E-18,2400,1

DOSE FROM YIELD = 1.8E+16 ATOMS/CM2

DEPTH          DIFFERENTIAL   ATOMIC % (FE)

 0              5.04E+21       5.94
 26.8           5E+21          5.89
 53.6           4.89E+21       5.77
 80.4           4.71E+21       5.56
 107.           4.47E+21       5.28
 134.           4.19E+21       4.94
 161.           3.86E+21       4.55
 188.           3.51E+21       4.13
 214.           3.14E+21       3.7
 241.           2.77E+21       3.26
 268.           2.4E+21        2.83
 295.           2.06E+21       2.43
 322.           1.74E+21       2.05
 348.           1.44E+21       1.7
```

The quality of the agreement between the data and the curve must be assessed manually by calculating the deviations and averaging them to produce a standard deviation. If there are N total data points of value $y_n(x)$ and the value from the computer-generated curve is $Y_n(x)$, then the standard deviation (S.D.) is

$$\text{S.D.} = \sqrt{\frac{\sum_{n=1}^{N} (Y_n - y_n)^2}{(N - 1)}} . \tag{20}$$

This will have the units of y_n, in this case photons per microcoulomb. For the unannealed case S.D. = 0.062 photon/microcoulomb, and for the annealed case S.D. = 0.076 photon/microcoulomb.

The subjective nature of this form of fitting curves to data is in the evaluation of the agreement in terms of shape. Except for the region beyond 15×10^3 microcoulombs in the annealed case, the agreement is good. This region of the annealed curve is probably in such poor agreement because of nonuniform diffusion such as grain-boundary-enhanced diffusion and distortions in sputter profiles when large sputtering charges are accumulated.

The profiles thus obtained are plotted in figure 2 as atomic percent nickel in iron versus depth. Note from tables 2 and 3 that the conversions are done by the computer and the correction factors are automatically applied.

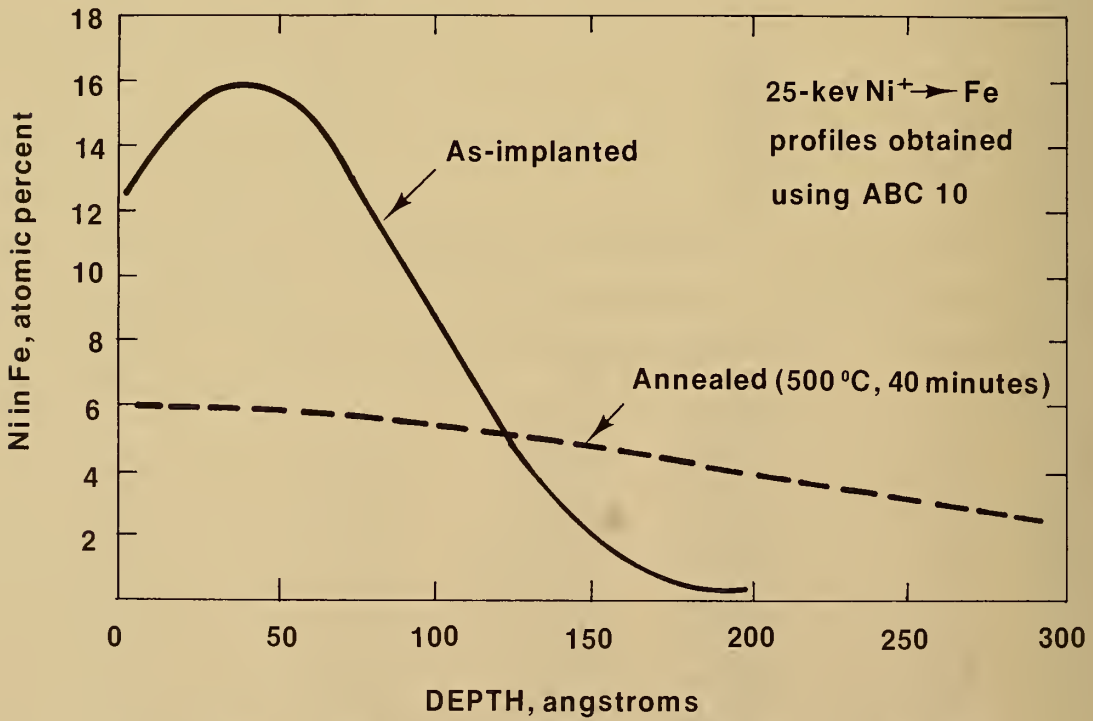

FIGURE 2. - Profiles obtained for nickel implanted into iron at 25 kev as obtained using ABC10.

As a check on the use of ABC10, it has been utilized to profile a sample whose profile has been well studied. A sample of arsenic-implanted silicon has been profiled, and the values of range and range straggle obtained agree reasonably well with those obtained by other experimenters (10, 13) and those predicted by LSS theory, considering the approximate nature of LSS theory when applied to polycrystalline materials and considering the experimental errors involved. These values are shown in table 4.

TABLE 4. - Values of range and range straggle for 30-kev As^+ implanted into silicon as determined from data of Ludvik (13), LSS theory (12), Iwaki (10), and the PIXE-IS technique using ABC10

	Range, A	Range straggle, A
PIXE-IS.....	260	180
LSS.....	212	83
Ludvik, et al.....	210	210
Iwaki.....	210	75

CONCLUSIONS

It has been shown that ABC10 can be a useful tool for interpreting integral Gaussian profiles, particularly for ion-implanted metals. The program utilizes manual fitting of integral profiles with range, range straggle, and diffusion coefficient as parameters resulting in Gaussian or diffused Gaussian (Fick's law) profiles. The program takes account of X-ray absorption and proton energy loss and includes conversion factors that can result in a quantitative profile.

REFERENCES

1. Abramowitz, M., and I. A. Stegun. Handbook of Mathematical Functions. Dover Press, New York, 1965, p. 299.

2. Andersen, H. H., and J. F. Ziegler. Hydrogen Stopping Powers and Ranges in All Elements. Pergamon Press, New York, 1977, 317 pp.

3. Churchill, R. V. Fourier Series and Boundary Value Problems. McGraw-Hill Book Co., New York, 1963, p. 156.

4. Covino, B. S., Jr., P. B. Needham, Jr., and G. R. Conner. Anodic Polarization Behavior of Fe-Ni Alloys Fabricated by Ion Implantation. J. Electrochem. Soc., v. 125, No. 3, March 1978, pp. 370-372.

5. Covino, B. S., Jr., B. D. Sartwell, and P. B. Needham, Jr. Anodic Polarization Behavior of Fe-Cr Surface Alloys Formed by Ion Implantation. J. Electrochem. Soc., v. 125, No. 3, March 1978, pp. 366-369.

6. Crank, J. The Mathematics of Diffusion. University Press, New York, 1957, 259 pp.

7. Fox, A. H. Fundamentals of Numerical Analysis. Ronald Press, New York, 1963, p. 58.

8. General Services Administration Computer Time-Sharing Service. Applications Library Operating Instructions. Federal Data Processing Center, Atlanta, Ga., August 1973, 358 pp.

9. Henke, B. L., and E. S. Ebisu. Low Energy X-Ray and Electron Absorption Within Solids (100-1500 eV Region). Ch. in Advances in X-Ray Analysis, v. 17, ed. by C. L. Grant, C. S. Barrett, J. B. Newkirk, and C. O. Rund. Plenum Press, New York, 1974, pp. 150-213.

10. Iwaki, M., K. Gamo, K. Masuda, S. Namba, S. Ishihara, and I. Kimurd. Concentration Profiles of Arsenic Implanted in Silicon. Ch. in Ion Implantation in Semiconductors and Other Materials, ed. by B. L. Crowder. Plenum Press, New York, 1973, pp. 111-118.

11. Khan, J. M., D. L. Potter, and R. D. Worley. Proposed Method for Microgram Surface Density Measurements by Observation of Proton-Produced X-Rays. J. Appl. Phys., v. 37, No. 2, February 1966, pp. 564-567.

12. Lindhard, J., J. M. Scharff, and H. E. Schiott. Atomic Collisions, II. Range Concept and Heavy Ion Ranges. Kgl. Danske Vid. Selsk., Matt-Fys. Medd., v. 33, No. 14, 1963, pp. 42-52.

13. Ludvik, S., L. Scharpen, and H. E. Weaver. Measurement of Arsenic Implantation Profiles in Silicon Using an Electron Spectroscopic Technique. Ch. in Ion Implantation in Semiconductors, ed. by S. Namba. Plenum Press, New York, 1975, pp. 155-162.

14. Mayer, J. W., and E. Rimini. Ion Beam Handbook for Material Analysis. Academic Press, New York, 1977, p. 316.

15. Oechsner, H. Sputtering - A Review of Some Recent Experimental and Theoretical Aspects. Appl. Phys., v. 8, 1975, pp. 185-191.

16. Winterbon, K. B. Ion Implantation Range and Energy Deposition Distributions. Plenum Press, New York, v. 2, 1975, 341 pp.

APPENDIX.--LISTING OF ABC10

The following listing of ABC10 was obtained directly from storage in the GSA RAMUS system. Some of the symbols are defined in table 1.

```
100 REM ABC 10
110 PRINT
120 PRINT "IF R=0, RESET ALL.  IF R.S.=0, RESET STEP AND MAX. DEPTH."
130 PRINT
140 DIM U (10),R(10)
150 LET I=0
160 FOR I=1 TO 5
170 READ U(I),R(I)
180 NEXT I
190 GO TO 1310
200 PRINT "ENTER STEP SIZE, MAXIMUM DEPTH";
210 INPUT T6,V
220 LET L=0
225 FOR L=0 TO V STEP T6
230 LET A0=L
240 LET B0=1.25*V
250 LET N0=50
260 IF L=0 THEN 1170
270 LET X=X
320 LET A1=.34802
330 LET A2=-.09588
340 LET A3=.74786
350 IF T=0 THEN 720
360 DEF FNE(Y,Z)=(A1*Y+A2*Y↑2+A3*Y↑3)*EXP(-1*Z↑2)
370 LET B2=1+((2*D*T)/((C↑2)*1E-16))
380 LET B1=1/(2*(C↑2)*B2)
390 LET B3=(1E-8)/(2*SQR(D*T)*SQR(B2))
400 LET B4=((D*T*B)*1E8)/((C↑2)*SQR(D*T)*SQR(B2))
410 LET B5=A/(2*SQR(B2))
420 LET X4=-1*B3*X-B4
430 LET X5=B3*X-B4
440 LET U4=EXP(-1*B1*(X-B)↑2)
450 LET U5 =EXP(-1*B1*(X+B)↑2)
460 IF X4<0 THEN 560
470 IF X5<0 THEN 620
480 IF X4>0 THEN 680
490 IF X5<0 THEN 530
500 LET T2=1/(1+.47047*X5)
510 LET U7 =FNE(T2,X5)
520 LET U2=U5*U7
530 LET Y=G*B5*(U1+U2)
535 IF E=1 THEN 1430
550 GO TO 790
560 LET X4=-1*X4
570 LET T1=1/(1+.47047*X4)
580 LET U6 =2-FNE(T1,X4)
590 LET U1 =U4*U6
600 LET X4=-1*X4
610 GO TO 470
620 LET X6=-1*X5
630 LET T2=1/(1+.47047*X5)
640 LET U7 =2-FNE(T2,X5)
650 LET U2=U5*U7
660 LET X5=-1*X5
670 GO to 480
680 LET T1=1/(1+.47047*X4)
690 LET U6 =FNE(T1,X4)
700 LET U1=U4*U6
```

```
710 IF X4>0 THEN 530
720 LET B2=1+((2*D*T)/((C↑2)*1E-16))
730 LET B1=1/(2*C↑2*B2)
740 LET B5=A/2
750 LET U1=2*EXP((-1*B1)*(X-B)↑2)
760 LET U2=0
770 GO TO 530
790 IF J=1 THEN 980
800 IF J=2 THEN 1020
810 LET A8=A0
820 LET Z0 = 0
830 LET D8=(B0-A0)/N0
840 LET B8=A8
850 LET B8=B8+D8
860 IF B8<=B0 THEN 890
870 IF Z0>0 THEN 1070
880 LET B8=B0
890 LET C1=.5*(B8+A8)
900 LET C2=B8-A8
910 LET S=0
920 LET I=0
930 LET I=I+1
940 LET W=C2*J(I)
950 LET X=C1+W
960 LET J=1
970 GO TO 270
980 LET S=S+R(I)*Y
990 LET X=C1-W
1000 LET J=2
1010 GO TO 270
1020 LET S=S+R(I)*Y
1030 IF I<5 THEN 930
1040 LET Z0 =Z0 + S*C2
1050 LET A8=B8
1060 GOTO 850
1070 IF L=0 THEN 1270
1080 LET Q=Z0+M
1085 LET Q6=(V-L)/2
1086 LET Q7=EXP(-1*Q6*Q8*K)
1087 LET G4=((G3=(G1*K*Q6))/G3)↑G2
1090 PRINT L,Q*Q7*G4
1100 LET J=0
1110 IF Z0<(P/1E4) THEN 220
1120 IF (V-L)<T6 THEN 1460
1130 NEXT L
1140 DATA 744371695E-10,147762112E-9,216697697E-9,134633360E-9
1150 DATA 339704784E-9,109543181E-9,432531683E-9,747256746E-10
1160 DATA 486953264E-9,333356722E-10
1170 PRINT
1180 PRINT "ENTER R,R.S.,D,T,&1 FOR PROFILE";
1190 INPUT B,C,D,T,E
1200 IF B=0 THEN 1310
1210 IF C=0 THEN 200
1220 IF E=1 THEN 1380
1230 PRINT
1240 PRINT "DEPTH","INTEGRAL"
```

```
1250 LET G=1
1255 LET A=1
1260 GO TO 270
1270 LET H6=EXP(-1*Q8*K*(V/2))
1272 LET H7=((G3-(G1*K*(V/2)))/G3)↑G2
1273 IF E=1 THEN 1384
1275 LET G-(P-M)/(Z0*H6*H7)
1280 SET DIGITS 3
1290 PRINT L,P
1300 GO TO 1100
1310 PRINT "ENTER VALUE OF INTEGRAL AT 0 AND AT INFINITY";
1320 INPUT P,M
1325 IF M> P THEN 1310
1345 PRINT "ENTER X-RAY ABSORPTION FACTOR (ANG.-1)";
1346 INPUT Q8
1347 PRINT "ENTER STOPPING POWER (EV/ANG.), POWER FACTOR, AND E0 (EV)"
1348 INPUT G1,G2,G3
1360 PRINT "ENTER CONV. FACTORS: A/K AND A/C/P/MIC.";
1370 INPUT K,H
1375 GO TO 200
1380 SET DIGITS 3
1381 PRINT
1382 GO TO 1270
1384 PRINT "DOSE FROM YIELD =";H*(P-M)/H6*H7);"ATOMS/CM2"
1385 PRINT
1386 PRINT "DEPTH","DIFFERENTIAL","ATOMIC %(FE)"
1387 PRINT
1388 LET C6=(2-FNE((1/(1+(.47047)*(B/(1.414*C))))),(B/(1.414*C))))
1389 LET A=H*(P-M)/(H6*H7*2.5066E-8*C*K*C6)
1390 LET G=1
1400 FOR X=0 TO V STEP T6
1415 GO TO 320
1430 PRINT X*K,Y,100*(Y/8.48E22)
1440 IF X=V GO TO 1170
1450 NEXT X
1460 LET L=0
1470 GO TO 220
1480 END
```

PD 18

INT.-BU.OF MINES,PGH.,PA. 24272

DOBBS BROS.
LIBRARY BINDING
DEC 80
ST AUGUSTINE
FLA.
32084

LIBRARY OF CONGRESS
0 002 960 021 1